Infinite Dilution Activity Coefficients and P-x Data for Aqueous and Nonaqueous Binary Systems using an Isothermal Equilibrium Static Cell

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Vapor-liquid equilibrium data are important for estimating equipment size in the design of unit operations in chemical engineering, especially separation and purification processes. Direct determination of activity coefficients at infinite dilution for engineering design calculations gives reliable results, is cost effective, and can result in significant enhancements to separation equipment efficiency.

This paper investigates vapor-liquid equilibrium (VLE) data and behavior by directly determining isothermal activity coefficients at infinite dilution for five aqueous and one nonaqueous binary mixtures using an equilibrium static-cell apparatus [1]. The aqueous binary systems consist of pure water and the following chemical solutes: isopropyl alcohol, acetone, 1,2-dichloroethane, methyl ethyl ketone (MEK), and toluene. A binary mixture of isopropyl alcohol and acetone represents the nonaqueous binary system. Experiments are done in an equilibrium static-cell apparatus in the dilute region of each constituent (less than 1.0 mole % solute) at 25 °C to determine activity coefficients at infinite dilution γ^{∞}. Binary interaction parameters (BIPs) for the NRTL (nonrandom two-liquid) activity coefficient model are determined from the experimental values of γ^{∞} for these binary mixtures. Subsequently, predictions of VLE behavior (T-P-xi-yi) of these binary systems, based on the new set of BIPs, are compared with experimental data and other published predictions.

KEY WORDS: Activity Coefficients, Infinite Dilution, Organic-Water Mixtures, Vapor-Liquid Equilibria, NRTL Model